Constraints on transmission, dispersion, and density of states in dielectric multilayers and stepwise potential barriers with arbitrary layer arrangement

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Normal-incidence transmission and dispersion properties of optical multilayers and one-dimensional stepwise potential barriers in the non-tunneling regime are analytically investigated. The optical paths of every constituent layer in a multilayer structure, as well as the parameters of every step of the stepwise potential barrier, are constrained by a generalized quarter-wave condition. No other restrictions on the structure geometry is imposed, i.e., the layers are arranged arbitrarily. We show that the density of states (DOS) spectra of the multilayer or barrier in question are subject to integral conservation rules similar to the Barnett-Loudon sum rule but ocurring within a finite frequency or energy interval. In the optical case, these frequency intervals are regular. For the potential barriers, only non-periodic energy intervals can be present in the spectrum of any given structure, and only if the parameters of constituent potential steps are properly chosen.

The integral conservation relations derived analytically have also been verified numerically. The relations can be used in dispersion-engineered multilayer-based devices, e.g., ultrashort pulse compressors or ultracompact optical delay lines, as well as to design multiple-quantum-well electronic heterostructures with engineered DOS.

I. INTRODUCTION

Over the centuries, the concept of homogeneity has played a major part in both mathematics and physics. The very name of a fundamental monograph on electrodynamics [1], *Electrodynamics of Continuous Media*, suggests that there should also exist electrodynamics of *discontinuous* media, quite distinct and yet unexplored. Indeed, most real-world physical phenomena and processes are usually neither continuous nor homogeneous, and all seemingly homogeneous substances are in fact discontinuous on the molecular and atomic level. The reason why the concept of homogeneous media is applicable and produces good results in electrodynamics is that, in the first place, the microscopic structure is so much smaller than typical electromagnetic wavelengths that an effective-medium approximation is valid. Secondly, many macroscopic systems can be broken up into several homogeneous parts, the relatively large size of which making the studies of the whole system comparatively simple.

The intermediate case of *mesoscopic structures* where inhomogeneities appear on the scale not minuscule enough to use an effective-medium approach but not too large to allow finite-size effects to be neglected has appeared more or less recently. This was largely motivated by the advancement of technology, allowing such structures to be fabricated and characterized. Even the first steps in this direction have already caused major advancements. The onset of semiconductor heterostructures was a breakthrough in electronics, the pioneers in the area awarded the Nobel Prize in 2000 [2]. The introduction of quantum mesoscopic systems such as nanocrystals and quantum dots opens new horizons in many areas, including biological sensor design and solid-state quantum computation (see, e.g., [3] and references therein). The introduction of micro- and nanostructured optical materials has opened up whole new areas of photonic crystal research, integrated optics, and the newly-emerging metamaterial physics (see [4]), with innumerable applications in telecommunication.

It appears that by arranging the matter in a mesoscopically structured fashion, one can engineer its properties (e.g., electronic and/or optical) with considerable freedom. One can achieve as rich a variety as seen among natural substances due to a known diversity in their molecular-sized chemical composition. This freedom is especially increased when the concept of structuring is extended beyond periodicity (see the recent review [5]), such as in quasiperiodic [6] or fractal media [7]. Often it is even possible to design a structured medium in order to achieve the chosen desired properties [8, 9]. Structured media can even exhibit optical properties beyond what occurs in natural materials, e.g., negative refraction [10] and the ability to slow down or stop light pulses [11].

All physical phenomena that involve interaction between light and matter appear to be altered in inhomogeneous media. This alteration is believed to be a fundamental physical principle involving modification of the properties of the vacuum (electromagnetic or electronic) in the vicinity of inhomogeneities. Such modification is generally described using the concept of the density of states (DOS) [12]; however, this concept is not without discussion points as regards definition of the DOS in finite vs. infinite media [13]. Despite those difficulties, the DOS concept appears a promising candidate for a universal approach towards consistent description of physical processes in arbitrarily inhomogeneous media.

As an example, it should be clear that the above mentioned modification of the vacuum cannot be totally arbitrary. Causality had been shown to restrict the modification of spontaneous emission rate by spectral redistribution with the total emission rate remaining unaffected (the Barnett-Loudon sum rule [14]). Since spontaneous emission is related to the DOS, this rule can be expressed as impossibility to change the total "number" of states, but only to redistribute them spectrally, which appears to be intuitively clear and heuristically potent.

In this paper we report on another, related limitation con-

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cerning the modification of transmission and dispersion properties of optical dielectric multilayers as well as of electronic heterostructures consisting of stepwise potential wells and barriers in the non-tunneling regime.

For the optical case, making all constituent layers commensurate in optical path produces a set of equidistant single-layer reflection-free (SLRF) points $2m\omega_0$ where (and only where) the dispersion relation of the structure coincides with that of a homogeneous medium (i.e., $k(2m\omega_0) \propto 2m\omega_0$). We have found that the optical DOS integrated between these points does not depend on the structure geometry and does not change if the constituent layers (whose optical paths are commensurate with respect to each other) are rearranged. The degree of modification to the optical properties as due to inhomogeneity of the structure is thus shown to be limited not only in its amount but also in its extent. This means that not only is a DOS enhancement in one spectral region compensated for in some other region, but also the compensation must occur within the distance $2\omega_0$ between the SLRF points, which is a spectral interval preset by the structural parameters of the constituent element.

For the stepwise potential, similar relations have been shown to exist. The single-layer reflection-free points do occur but are no longer equidistant. For any given values of parameters for constituent elements, there can be either none or a multitude of aperiodically located SLRF points for all structures. In the latter case, the integral constraints on the DOS can still be obtained, but they are more complex. In both optical and quantum case, the analytical relations obtained have been confirmed in numerical calculations.

The paper is organized as follows. In Sec. II we introduce the reader to the structures under study and provide the necessary basic notation. In Sec. III, we discuss the concept of the DOS and its relation to the spectral properties of the structure. In Secs. IV and V we derive the constraints on the DOS for optical multilayers and for binary stepwise potential barriers, respectively. In Sec. VI the results obtained in the previous sections are compared and discussed. Finally, Sec. VII summarizes the paper.

II. OPTICAL AND ELECTRONIC HETEROSTRUCTURES

We start by considering a one-dimensional dielectric multilayer nanostructure of N layers, each layer having a thickness d_j and a refractive index n_j, infinite in the transverse directions and surrounded on both sides by free space ($n_0 = 1$). Consider a normally incident plane monochromatic wave propagating through such a structure. This problem is one-dimensional, and unless the multilayer structure contains optically anisotropic materials, it can be described using scalar electric field governed by the scalar Helmholtz equation [4]

$$\frac{\partial^2}{\partial x^2}E(x) + \varepsilon(x)\frac{\omega^2}{c^2}E(x) = 0. \tag{1}$$

Let $R(\omega)$ and $T(\omega)$ denote the complex (i.e., taking into account the phase shift) reflection and transmission coefficients of the multilayer structure, respectively. Let us now assume that all the layers have such parameters that the optical path $n_j d_j$ is the same for any j, so that

$$n_1 d_1 = n_2 d_2 = \cdots = n_j d_j = \cdots = n_N d_N \equiv \pi c/2\omega_0. \tag{2}$$

where ω_0 is defined as the *central frequency*. We call any structure that conforms to Eq. (2) the *quarter wave* (QW) multilayer structure.

It can be shown that for any even multiple of ω_0 the propagating wave passes each constituent layer without reflection (no internal reflections at the layer interfaces), and thus gains the phase shift $\Delta\varphi = \frac{\omega}{c} n_j d_j$, which is the same for all layers in view of the QW condition as expressed with Eq. (2). (See also [15] for more detail on phase relations in Fresnel reflection from one layer.) As a result, the structure becomes fully transparent ($|T(2m\omega_0)| = 1$) regardless of the number or arrangement of constituent layers, and the total phase shift becomes a simple sum of the shifts for all the layers:

$$T(\omega_m = 2m\omega_0) = \exp\left[\mathrm{i}\frac{\omega}{c}\sum_{j=1}^{N} n_j d_j\right] = \exp\left(\mathrm{i}Nm\pi\right). \tag{3}$$

Eq. (3) essentially provides a set of equidistant frequency points [we will call them *single-layer reflection-free* (SLRF) points] where the propagation phase (and hence, the wave number) is linearly dependent on frequency regardless of the structure. Indeed, the dispersion relation at these points ($D = \sum_{j=1}^{N} d_j$)

$$k_m(\omega_m) = k(2m\omega_0) = \frac{Nm\pi}{D} = \frac{N\lambda_0}{2D}\frac{\omega_m}{c} \tag{4}$$

linearly relates k_m and ω_m, as is the case for a homogeneous medium. This linear dependence occurs only at the set of SLRF points $\omega_m = 2m\omega_0$, and Eqs. (3)–(4) are not true anywhere between these points. Note that among all the transmission resonances present in a given multilayer's spectrum, the SLRF points represent stationary waves without any correlations on a length scale greater than the optical path of one constituent layer. As such, they are naturally the least localized non-evanescent eigenstates possible in any given QW multilayer.

Moreover, QW structures are known to possess spectral periodicity in transmittance [16]

$$|T(\omega + 2m\omega_0)| = |T(\omega)| \tag{5}$$

and mirror symmetry within each period [16]

$$\begin{gathered}|T\left((2m+1)\omega_0 + \omega\right)| = |T\left((2m+1)\omega_0 - \omega\right)|, \\ 0 < \omega < \omega_0.\end{gathered} \tag{6}$$

Now let us note that Eq. (1) is isomorphic to the Schrödinger equation governing a quantum particle with mass m_p and energy E_p in a stepwise potential $u(x)$

$$\frac{\hbar^2}{2m_p}\frac{\partial^2}{\partial x^2}\psi(x) + \left[E_p - u(x)\right]\psi(x) = 0 \tag{7}$$

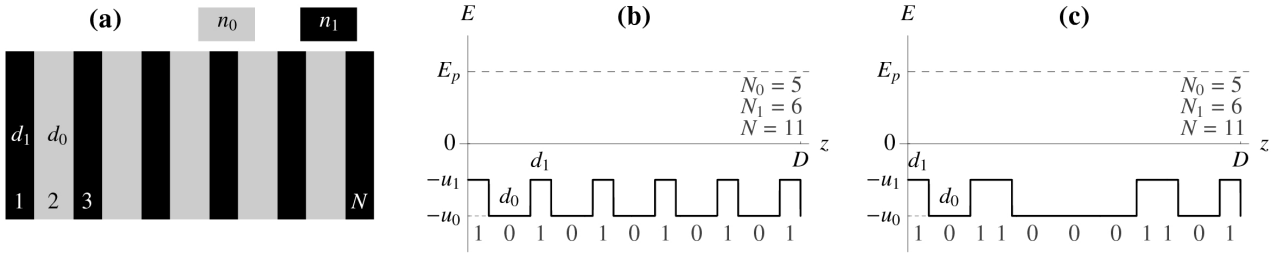

Figure 1: A binary optical multilayer **(a)** together with its quantum mechanical counterpart: a particle with energy $E_p = \hbar\omega$ in 1D periodic **(b)** and non-periodic **(c)** binary stepwise potential.

If the potential function is a constant ($u(x) = -u_0$), the solution of Eq. (7) is a plane-wave function

$$\psi_0(x) = \exp \mathrm{i}kx = \exp\left[\mathrm{i}\left(\frac{\sqrt{2m_p}}{\hbar}\sqrt{E_p + u_0}\right)x\right], \quad (8)$$

which is analogous to a plane optical wave with the wave vector $k = \left(\sqrt{2m_p}/\hbar\right)\sqrt{E_p + u_0}$. If $E_p > u(x)$ for any x, then k is real and the particle interacts with a potential barrier in the non-tunneling (Ramsauer) regime. This is a quantum mechanical analogy to electromagnetic wave propagation in a dielectric structure. Similar to the optical case, one can consider a stepwise potential barrier consisting of N "elementary wells" (Fig. 1b,c). The role of refractive index is taken by the potential energy u_j in every step of the whole potential function. The frequency is replaced by the particle energy E_p, which can be expressed in terms of de Broglie frequency [17] as $E_p = \hbar\omega$. The case $E_p < u(x)$, which causes imaginary wave vector in Eq. (8), is the tunneling case analogous to light propagation in absorbing media (e.g., metals). It is outside the scope of the present paper. To assure $E_p > u(x)$, let us assume $E_p \geq 0$ and $u(x) < 0$ from now on.

Furthermore, it is commonly known that if the potential represents a single step ($u(x) = -u_0$ for, say, $x < x_0$ and $u(x) = -u_1$ otherwise), one can introduce the coefficients

$$r_{01} = \frac{k_0 - k_1}{k_0 + k_1}, \quad t_{01} = \frac{2k_0}{k_0 + k_1}, \quad (9)$$

which, when squared, denote the probability of finding the impinging quantum particle reflected or transmitted, respectively [17]. One can name them the reflection and transmission coefficient for matter waves, a potential step corresponding to a single interface between dielectric media. Since the expressions for r and t are the same (the wave vector k taking the role of refractive index), one can use the same transfer-matrix formalism for determining both the stationary electromagnetic wave distribution in a multilayer [18] and the steady-state wave function for quantum particles travelling through a complex stepwise potential [19]. Note that Eq. (8) indicates that the "refractive index" introduced in this way possesses an inherent quadratic dispersion.

Finally, we call a multilayer structure *binary* if it can be represented as consisting of two types of constituent layers (denoted as binary digits 0 and 1, following the notation in [20]), to which two combinations of refractive index and thickness $(n_0; d_0)$ and $(n_1; d_1)$ are attributed. By arranging the 0's and 1's in different sequences, it is possible to vary the geometry of the structure very widely, making it periodic (if 0 and 1 alternate, as in 10101010101), disordered (if the sequence is randomly determined), or deterministically aperiodic (e.g., quasiperiodic [6] or fractal [7]). A binary potential barrier, with constituent elementary wells associated with $(u_0; d_0)$ and $(u_1; d_1)$, can be introduced likewise. For brevity, we will occasionally use the term "layers" for both types of constituent elements.

Note that whenever the sequence contains two identical layers (e.g., "00" in 1010100101), it will of course mean in practice that the corresponding structure will contain a single layer with thickness $2d_0$. However, for the purpose of this work we will regard such combinations as two separate constituent layers. The number of layers of both types N_0 and N_1, as well as their total number $N = N_0 + N_1$, will then remain the same regardless of layer rearrangement, indicative of the transmission coefficient phase at the SLRF points [see Eq. (3)].

III. OPTICAL AND QUANTUM DENSITY OF STATES

As mentioned in Section I, any inhomogeneity present in space is known to modify the properties of the quantum or electromagnetic vacuum in its vicinity. This modification takes the form of the change in the local DOS. It is believed to affect all phenomena that involve light-matter interaction, such as spontaneous emission or Raman scattering (see, e.g., [12] and references therein).

Physically, the local DOS $\mathcal{N}(\mathbf{r}, E)$ is directly related to the trace of Green's function for the system in question: $\mathcal{N}(\mathbf{r}, E) \propto \mathrm{Im\,Tr}\, G(\mathbf{r}, \mathbf{r}, E)$. By taking the integral Green's function $G(E)$ in place of the local one, one obtains the value of the DOS $\mathcal{N}(E)$ that is characteristic to the whole system for a given value of energy. In a spatially finite system (a potential well with infinite walls or a closed resonator), only the states with a discrete set of energy (or frequency) eigenvalues are allowed. Supposing that these eigenvalues are dense enough, this integral DOS has a rather loose mathematically but very intuitive meaning of the number of these discrete states per unit energy.

In an open resonator, any value of energy corresponds to an eigenstate, and the DOS transforms into a continuous spectrum $\mathcal{N}(E)$, indicative of spectral characteristics for the over-

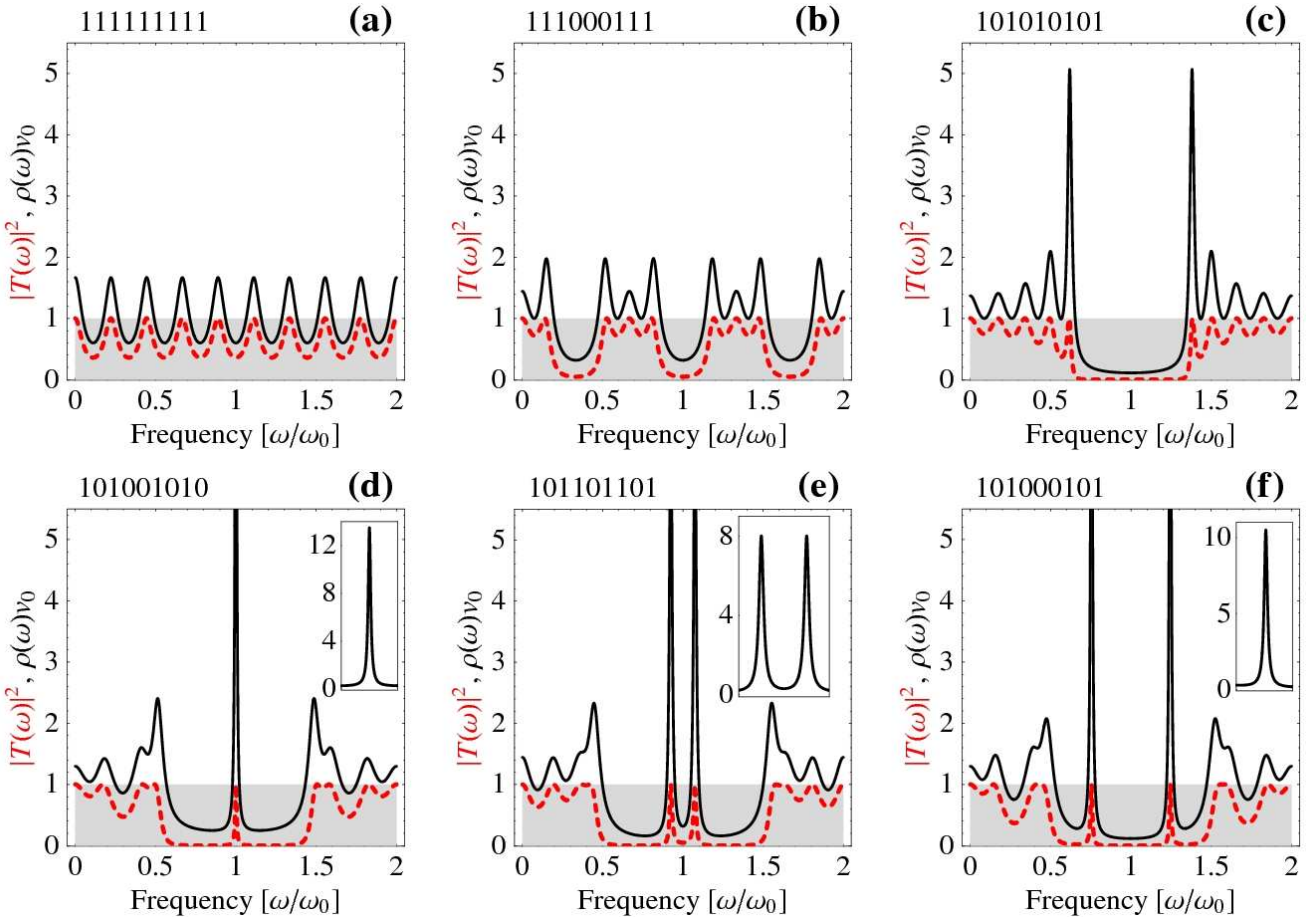

Figure 2: (Color online) Transmittance $|T(\omega)|^2$ (dashed line) and normalized averaged local DOS $\rho(\omega)v_0$ [as of Eqs. (15) and (18), solid line] for multilayer structures of different geometry: (a) single $9d_1$-thick layer; (b) 3-layer structure; (c) 9-layer periodic structure; (d) Fabry-Pérot-like periodic structure with a half-wave defect; (e) coupled-defect structure; (f) fractal Cantor-like structure. All multilayers have $N = 9$. The vertical scale is chosen alike for all plots for the ease of comparison, the insets showing the scale of clipped peaks. The area $[0, 1]$ is shaded to show the allowed region for transmittance, as well as to provide a visual guide for estimating the integral of $\rho(\omega)$ [see Eq. (19)].

all vacuum modification. It had been shown [21, 22, 23] that a finite-sized inhomogeneous potential located in an infinite 1D space causes the local DOS integrated over the whole space to undergo an overall finite modification $\Delta\mathcal{N}(E) \equiv \int_{-\infty}^{\infty} [\mathcal{N}(x, E) - \mathcal{N}_0(x, E)]\,\mathrm{d}x$. Note that we are considering a finite-sized inhomogeneity in an infinite space (an open resonator), as opposed to a finite system isolated from the outside space (a closed resonator). In the former, $\Delta\mathcal{N}$ was found to be proportional to the derivative of the total phase accumulated by the wave packet during its transmission through the inhomogeneity:

$$\Delta\mathcal{N}(E) = (1/\pi)\,(\mathrm{d}\varphi/\mathrm{d}E)\,, \tag{10}$$

which, as seen from Eq. (8), becomes asymptotically zero for very large energies compared to the potential (i.e., if nothing gets in the particle's way). A similar expression can be used to determine the local density of electromagnetic states, also called the optical DOS (for details on its definition in 2D and 3D case, see Refs. [13, 24]). The transition from local to integral DOS can be made in a similar manner to the quantum system. In the 1D case (the wave propagation in a multilayer is a 1D problem when only normal-incidence states are taken into account) the modification to the optical DOS $\Delta\mathcal{N}(\omega)$ is also likewise related to the derivative of transmission phase [25]:

$$\Delta\mathcal{N}(\omega) = (1/\pi)\,(\mathrm{d}(\varphi - \varphi_0)/\mathrm{d}\omega)\,. \tag{11}$$

The subtraction of the free-space phase shift φ_0 ensures that $\Delta\mathcal{N}(\omega) = 0$ in free space. In the work by Barnett and Loudon [14] it has been shown that the modification of spontaneous emission rate Γ by inhomogeneous medium (as compared to the free-space emission rate Γ_0) integrated over the whole spectrum must be zero (the Barnett-Loudon sum rule):

$$\int_0^{\infty} \left[\frac{\Gamma(\mathbf{r}, \omega)}{\Gamma_0(\omega)} - 1\right] \mathrm{d}\omega = 0. \tag{12}$$

The emission rate Γ is proportional to the local DOS $\mathcal{N}$, and the local optical DOS is frequency independent in free space (see [12]). Spectral integration in Eq. (12) can be interchanged with spatial integration over $\Gamma(\mathbf{r}, \omega)$. Hence, a similar relation

holds for the integral DOS:

$$\int_0^\infty \Delta\mathcal{N}(\omega)\mathrm{d}\omega = 0. \tag{13}$$

The transition from local to integral DOS, as well as the transition from $\Delta\mathcal{N}$ to $\mathcal{N}$, involves renormalization and therefore may be ambiguous. A simple way to counter the divergence is to accompany the transition from $\varphi - \varphi_0$ to φ with normalizing the DOS by the total thickness of the inhomogeneous medium D (see [26]):

$$\rho(\omega) \equiv \pi\frac{\Delta\mathcal{N}(\omega)}{D} = \frac{1}{D}\frac{\mathrm{d}\varphi}{\mathrm{d}\omega}, \tag{14}$$

The authors in [26] simply define ρ as the optical DOS without going into further details. We can see that it is in fact neither local nor integral, but rather has the meaning of *local DOS modified by a finite inhomogeneity, averaged in infinite 1D space*. In the absence of any inhomogeneity, Eq. (14) gives $\rho(\omega) = 1/c$, a known value for the DOS in 1D free space.

Further, Eq. (14) can be used to calculate $\rho(\omega)$ from the complex transmission coefficient $T(\omega)$ as

$$\rho(\omega) = \frac{[\mathrm{Im}\,T(\omega)]'\,\mathrm{Re}\,T(\omega) - \mathrm{Im}\,T(\omega)\,[\mathrm{Re}\,T(\omega)]'}{D\,|T(\omega)|^2}, \tag{15}$$

the derivation taken with respect to ω.

One must realize that the concept of the DOS introduced as in Eqs. (10)–(11), and especially, as in Eq. (14), is not without controversy. Questions arise already as to the physical meaning of the quantities involved. For example, one can define a "wave number" k *a posteriori* from the phase of the transmitted wave

$$k(\omega) = \frac{\varphi}{D} = \frac{\mathrm{Arg}\,T(\omega)}{D}, \tag{16}$$

which would equal the actual wave number in a homogeneous medium, or the Bloch wave number in a periodic multilayer at transmission resonances [26]. In such special cases, ρ would equal the inverse group velocity ($\rho(\omega) = (\mathrm{d}\omega/\mathrm{d}k)^{-1}$), the latter also equal to the energy velocity.

In the general case of non-periodic structures, however, the concepts of phase, group, and energy velocity, as well as their mutual correspondence, need to be re-examined. For instance, the "phase time" defined as $\mathrm{d}\varphi/\mathrm{d}\omega$ is, in general, not equal to the pulse's actual "dwell time" (see [25, 27]), although, admittedly, both have a similar frequency dependence and in some cases the phase time is a very good approximation for the dwell time [28]. That said, it is safer not to assign any direct physical meaning to k defined in Eq. (16) in the general case. We will thus treat it like a parameter within the scope of the present paper.

Another point is that the applicability of 1D models for electromagnetic problems is in general of limited value. The reason is that reduction of Maxwell's equations to the scalar wave equation (1), e.g., for multilayered media does not really make the problem entirely one-dimensional. In reality one deals with finite-width beams rather than plane waves and with excited atoms that can emit in any direction. The lateral width of the multilayers is finite, too. As pointed out in Ref. [29], the optical DOS reduces to the expression (14) only if off-axis wave propagation is totally left out.

That kept in mind, the function $\rho(\omega)$ nevertheless undergoes the same dramatic variation as does the transmittance itself when the structure geometry is varied (see Fig. 2). The peaks in $|T(\omega)|^2$ and $\rho(\omega)$ obviously correspond to each other. Note that this correspondence is a physical property of multilayers rather than just a mathematical property of Eqs. (14)–(15). Indeed, one can show analytically that $\rho(\omega) \propto |T(\omega)|^2$ for any single layer. This proportionality is due to the phase structure of the Airy formulas, and is obviously not there for arbitrary $\varphi(\omega)$ in Eq. (14). Numerical calculations confirm that spectral features in $|T(\omega)|^2$ and $\rho(\omega)$ also correspond for an N-layer structure, e.g., as seen in Fig. 2. It should be possible to show this analytically by induction but it is outside the scope of the present paper. We note instead that the same correspondence was observed in higher-dimensional systems (e.g., in slab photonic crystals [30]).

Besides, one can observe that the sharper is the transmission resonance around some frequency ω_r, the larger is the value of $\rho(\omega_r)$. Sharper transmission resonances correspond to stationary waves with greater energy localization, and it takes longer for greater energies to build up inside the structure. Hence, it takes longer for resonant transmission to manifest in such cases. Therefore the maxima of $\rho(\omega)$ are just those points where delayed light propagation is likely to be experienced. The DOS spectrum is thus valuable as a quick visual guide for determining the resonant behavior of any multilayer structure, as employed earlier [31].

Finally, let us note that although k in Eq. (16) cannot be assigned a direct physical meaning in the general case, it can be used as a parameter, which can provide some heuristic guidance in experiments on the group velocity dispersion-related effects (e.g., pertaining to propagation, compression, delay, and chirp compensation of ultrashort laser pulses). For some examples involving non-periodic structures, the reader is referred to Refs. [32, 33, 34].

IV. CONSTRAINTS IN MULTILAYERS

In the previous section, the use of $\rho(\omega)$ defined by Eq. (15) as a meaningful characteristic of the structure's optical properties has been motivated. It was demonstrated that $\rho(\omega)$ can be strongly modified by altering the geometry of the structure (Fig. 2). We proceed to show that the degree of geometry-induced modification imposed on ρ has fundamental limitations. One of these is the Barnett-Loudon sum rule – Eq. (13) holds both for the quantum mechanical and for the electromagnetic case when the corresponding expression for $\Delta\mathcal{N}(\omega)$ is used.

If the medium is a QW multilayer, the constraint becomes stricter and involves integration over *finite* rather than infinite frequency intervals. As the transmission properties in the SLRF points are given by Eq. (3), the integral of $\rho(\omega)$ between those points can be evaluated explicitly using Eqs. (16)

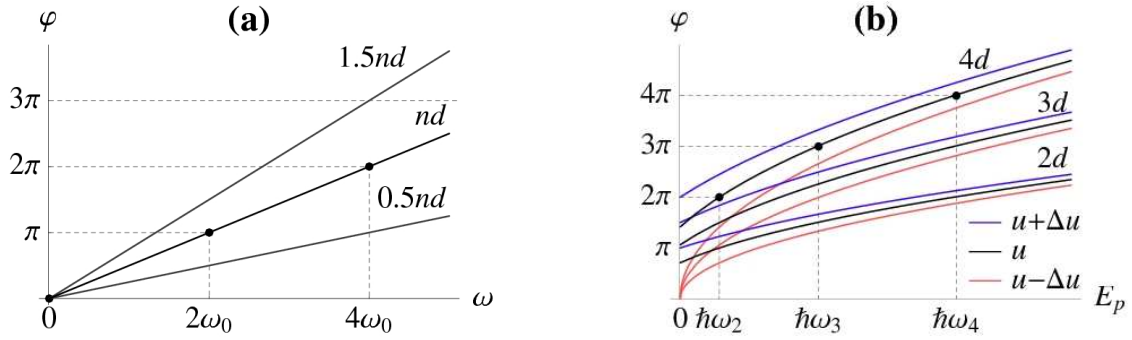

Figure 3: (Color online) The schematic frequency dependence of propagation phase for **(a)** optical waves [Eq. (23)] and **(b)** quantum wave function [Eq. (22)] in a slab of homogeneous dielectric and in a length of constant potential, respectively.

and (3)–(4) (see also [16]):

$$\int_{2m\omega_0}^{2(m+1)\omega_0} \rho(\omega)\mathrm{d}\omega = \int_{k[2m\omega_0]}^{k[2(m+1)\omega_0]} \mathrm{d}k = \frac{N\pi}{D}, \qquad (17)$$

which holds *regardless of the geometrical arrangement* of the constituent layers in the structure, provided that the layers obey the relation (2). One can further introduce the "bulk velocity prameter" from the minimum time it takes light to traverse the multilayer, internal reflections neglected, as

$$v_0 \equiv \frac{D}{\sum_j (d_j n_j/c)} = \frac{2\omega_0 D}{N\pi}. \qquad (18)$$

This is a parameter independent either of ω or of the layer arrangement of the structure. Making a transition to the dimensionless frequency $\eta \equiv \omega/\omega_0$ and taking into account the symmetry condition (6), we arrive at

$$\int_m^{m+1} v_0\rho(\eta)\mathrm{d}\eta = 1 \qquad (19)$$

and, further, since $v_0 = c$ and $\rho_0 = 1/c$ in free space,

$$\int_m^{m+1} \Delta\left[v_0\rho(\eta)\right]\mathrm{d}\eta = \int_m^{m+1} \left(v_0\rho(\eta) - c\rho_0\right)\mathrm{d}\eta = 0 \qquad (20)$$

for any integer $m \geq 0$.

The conditions (19)–(20) have no less a universal character than Eq. (13). They physically mean that the modification of the transmission or dispersion properties due to layer rearrangement in QW multilayers is only possible within a *finite* frequency range ω_0. One can see in Fig. 2 that despite apparently dramatic modification of $\rho(\omega)$, the enhancement in one portion of the spectrum appears compensated by a gap in another portion, so that the overall DOS, integrated between the SLRF points, remains unaffected. It is also important to realize that within ω_0, one can achieve *any* desired spectral shape, given the sufficient number of layers and sufficient freedom in their arrangement. For example, a heuristic optimization algorithm was recently used to demonstrate that certain aperiodic sequences can be employed to fabricate structures with desired spectral properties [9].

Note, too, the inverse proportionality between ω_0 and the optical path of the constituent layers. It follows that if the QW condition (2) is broken but the quantities $n_j d_j$ all remain commensurate, the same reasoning can be applied. Eqs. (17) and (19) can then be obtained by subdivision of the constituent layers, accompanied by the according increase in the central frequency ($\omega_0 \to N\omega_0$). In the limiting case of mathematically incommensurate layers, N goes to infinity, and the structure appears to possess the same freedom as a continuously inhomogeneous medium would, retaining only asymptotic relation

$$\lim_{N\to\infty} \frac{1}{N} \int_0^{N\omega_0} \rho(\omega)\mathrm{d}\omega = \frac{\pi}{D}, \qquad (21)$$

associated with increasing ω_0 to infinity in Eq. (20), and consequently, representing the sum rule (13).

V. CONSTRAINTS IN POTENTIAL BARRIERS

The concept of optical DOS appeared in electrodynamics largely by the influence of the quantum DOS. Such transfer of concepts makes use of the analogy between the Helmholtz (1) and Schrödinger (7) equations, as well as between a multilayer and a potential barrier, as outlined in Sec. II. In this section, we will attempt to make these analogies work backwards and determine if, and to what extent, the relation (17) can be generalized to the quantum mechanical case.

Consider a binary stepwise potential and the particle with mass m_p and energy $E_p \equiv \hbar\omega$ interacting with it in the nontunneling regime (Fig. 1b,c). Making use of the expression (8) for k, we can derive the frequency dependence for propagation phase of the particle's wave function for constant potential corresponding to one elementary potential well. Compared to the same dependence for an optical wave in a homogeneous slab corresponding to one constituent layer, it has the

form ($\alpha \equiv \sqrt{2m_p}/\hbar$)

$$\varphi^{(\mathrm{qm})}(\omega) \equiv k^{(\mathrm{qm})}(\omega)d = d\alpha\sqrt{\hbar\omega + u}; \quad (22)$$

$$\varphi^{(\mathrm{opt})}(\omega) = nd\omega/c. \quad (23)$$

Fig. 3 schematically shows both these dependencies. In the optical case (Fig. 3a) the only variable parameter is the slope given by nd. Hence, with the aid of Eq. (2) it becomes possible to achieve exactly the same dispersion relation, and hence the same set of SLRF points, for both constituent layers when $n_0 \neq n_1$. This is what forms the foundation for reasoning presented in the previous section. In the quantum case (Fig. 3b) u and d are seen to contribute in an essentially different way. Is is thus not possible to arrive at the same dispersion relation for two different potentials ($u_0 \neq u_1$).

However, one can still define a set of frequency points (though no longer equidistant) where $\varphi^{(\mathrm{qm})}(\omega_j) = j\pi$. In these points, as can be seen from Eqs. (8) and (9), the whole structure would be totally "transparent" for incoming quantum particles (the Ramsauer effect). If the structure is binary, the frequencies for both kinds of elementary wells are given by

$$\hbar\omega_{j_{0,1}}^{(0,1)} = j_{0,1}^2\pi^2/d_{0,1}^2\alpha^2 - u_{0,1}. \quad (24)$$

Since two different parabolic curves can still have intersection points, one can manage to achieve $\omega_{j_0}^{(0)} = \omega_{j_1}^{(1)}$ for two pairs of j_0 and j_1. The reasoning presented in the previous section can then be reproduced involving the quantity ρ defined exactly as in Eqs. (14) and (17) and having the same physical background. The dependence on ω, however, will be more complex due to inherent dispersion as seen in Eq. (8).

For simplicity and for the sake of further analogy between optical and quantum systems, let us require one of the equal frequency pairs in Eq. (24) to correspond to $\omega = 0$ (which is always true for optical waves where all dispersion curves pass trough the origin, see Fig. 3a). In this case we arrive at

$$\alpha^2 d_0^2 u_0 = \alpha^2 d_1^2 u_1 = j_{\mathrm{qw}}^2\pi^2, \quad (25)$$

which can be seen as a quantum analogy to the condition (2). The second pair (j_0, j_1) can then be found as an integer solution of the equation (first suggested in our earlier work [35])

$$j_0^2 - \left(1 - \beta/j_{\mathrm{qw}}^2\right) j_1^2 = \beta, \quad j_{0,1} > j_{\mathrm{qw}}; \quad \beta \equiv (u_0 - u_1)\alpha^2 d_0^2/\pi^2. \quad (26)$$

It can be seen that for any integer $j_{0,1} > j_{\mathrm{qw}}$ there is a rational β that solves Eq. (26). But β is related to the parameters of the constituent potential wells. So, the inverse problem, i.e, finding suitable $j_{0,1}$ for a given β, is far more interesting from a physical point of view. However, is not so straightforward and is mathematically related to finding Pythagorean triples in integer numbers. One can confirm numerically that there are a multitude of solutions for many rational values of β (see Table I). Some of them can be represented via recurrent relations, e.g., for $\beta = 1$ some of the solutions represent a series:

$$j_1^{(i+1)} = j_1^{(i)} + 6 + 4i, \quad j_0^{(i)} = j_1^{(i)} - 1, \quad (27)$$

where $j_1^{(0)} = j_{\mathrm{qw}}^{(\min)} = 2$. Other cases are more complex, but they, too, can be seen to form distinct solution branches (Fig. 4).

Once j_0 and j_1 have been found, an analogous relation to Eq. (17) can be formulated as

$$\int_{0=\hbar\omega_{j_{\mathrm{qw}}}}^{\hbar\omega_{j_0}^{(0)}=\hbar\omega_{j_1}^{(1)}} \rho(E)\mathrm{d}E = \frac{\hbar\pi}{D}\left[N_0(j_0 - j_{\mathrm{qw}}) + N_1(j_1 - j_{\mathrm{qw}})\right]. \quad (28)$$

Note that Eq. (28) is more complicated than its optical counterpart (17), and becomes, in general, dependent on the number of constituent potential wells $N_{1,2}$. This dependence cannot be eliminated because one sees from Eq. (26) that it is impossible to have $j_0 = j_1$ without violating the assertion that $j_{0,1} > j_{\mathrm{qw}}$. It is still, however, completely independent of layer rearrangement. In this sense, Eq. (26) represents a universal quantum mechanical conservation relation for the DOS over a finite energy interval.

To demonstrate the results numerically, we have considered a stepwise AlAs/GaAs quantum well ($\Delta u = 1000$ meV). To aim at $\beta = 4/5$, we have taken $d_0 = 21.2$ Å, $d_1 = 47.4$ Å, according to Eqs. (25)–(26). One possible solution of Eq. (26) would then be $j_{\mathrm{qw}} = 1$, $j_0 = 2$, $j_1 = 4$ (see Table I). The structures made of $N = 9$ elementary wells were used, and the numbers N_0 and N_1 were fixed, too, at the values 4 and 5, respectively.

We see in Fig. 5 that both $\rho(E)$ and the transmission $T(E)$ are subject to quite a strong modification. It resembles the modification seen in dielectric multilayers (compare, e.g., Fig. 5a,b with Fig. 2a,c). Two differences are the presence of a decaying background due to the inherent dispersion [see Eq. (22)] and the lack of periodicity because Eq. (2) can no longer be satisfied.

However, if we integrate $\rho(E)$ between the SLRF points ($\hbar\omega_{j_{\mathrm{qw}}} = 0$ and $\hbar\omega_{j_0} = \hbar\omega_{j_1} = 3.75$ eV) as provided by Eq. (26), we can see that the integral does not change when the layers are rearranged. Table II provides the results for nine different structures and for several upper integration limits. It can be seen that both below and above 3.75 eV the integrals vary from structure to structure. When, however, the correct integration limits are chosen, the difference vanishes and all integrals equal 19, which is the right-hand side of Eq. (28) for the chosen values of parameters.

VI. DISCUSSION

The equations (17)–(20) and (28) constitute the main result of this paper pertaining to optical and electronic heterostructures, respectively. In both cases, we are dealing with conservation of the DOS ρ integrated across a finite energy or frequency region. As discussed in Sec. III, ρ represents the averaged local DOS as modified by the presence of finite-sized inhomogeneous structure in an infinite 1D free space. It is related to the dispersion and the transmission properties of the heterostructures in question [see Eqs. (14)–(15)].

Table I: Some values of β that allow integer solutions of Eq. (26), along with some of such solutions obtained numerically.

$\beta < 1$	$(j_{\rm qw} : j_0, j_1)$	$\beta \geq 1$	$(j_{\rm qw} : j_0, j_1)$
1/4	$(1:13,15)$; $(1:181,209)$; $(2:122,126)$	1	$(2:7,8)$; $(2:26,30)$; $(3:17,18)$; $(3:99,105)$; $(4:31,32)$
1/3	$(1:9,11)$; $(1:89,109)$; $(2:90,94)$	3/2	$(2:8,10)$; $(2:68,86)$; $(3:63,69)$
1/2	$(1:5,7)$; $(1:29,41)$; $(2:58,62)$; $(3:207,213)$	2	$(2:10,14)$; $(2:58,82)$; $(3:45,51)$
2/5	$(1:7,9)$; $(1:55,71)$; $(2:74,78)$	4	$(3:7,9)$; $(3:18,24)$; $(4:14,16)$; $(4:52,60)$; $(5:23,25)$
2/3	$(1:3,5)$; $(1:11,19)$; $(2:42,46)$; $(3:153,159)$	6	$(3:9,15)$; $(3:33,57)$; $(4:16,20)$
4/5	$(1:2,4)$; $(1:5,11)$; $(1:13,19)$; $(2:34,38)$	10	$(4:8,12)$; $(4:32,52)$; $(5:35,45)$

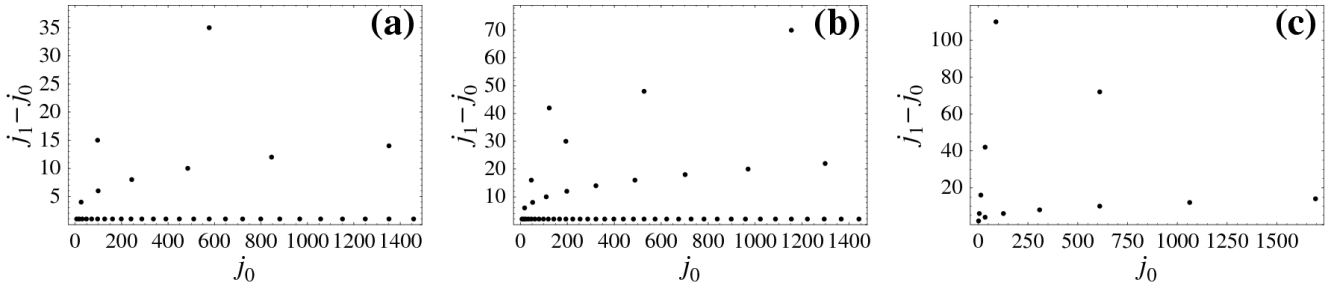

Figure 4: The distribution of integer solutions $j_{0,1}$ of Eq. (26) for **(a)** $\beta = 1$, **(b)** $\beta = 4$, and **(c)** $\beta = 4/5$. Distinct solution groups ("branches") can be seen.

These properties, as well as the DOS, can undergo dramatic modification as compared to those of homogeneous media (see Figs. 2 and 5) because a multilayer structure or a stepwise potential barrier can be very complex. Nevertheless, the modification appears to be limited both in its amount [see the right hand side of Eqs. (17) and (28)] and in its extent (by the finite integration limits in those equations).

There is an elegant physical explanation for the relations obtained. By engineering the geometrical properties of an inhomogeneous structure, it is only posible to redistribute the available electromagnetic or quantum states across the spectrum, but impossible to alter the "total number" of the states. The latter turns out to be related to the size or "1D volume" of the structure [as seen by the presence of N at the right-hand side of Eqs. (17) and (28)] and represents integrated characteristics of the structure-affected vacuum. So, an enhancement of the DOS in some pars of the spectrum (like the band edge resonances for a periodic structure in Fig. 2c) giving rise, e.g., to the spontaneous emission enhancement, is inevitably accompanied by a suppression of the DOS in other spectral region (like the band gap in the same figure), leading to the inhibition of light propagation and all phenomena involving light-matter interaction [4].

Table II: Numerically evaluated integrals $(D/\hbar\pi)\int \rho(E)\mathrm{d}E$ [as in Eq. (28)] from 0 to several upper energy values for nine structures with $N = 9$, $N_0 = 4$, and $N_1 = 5$ (same as in Fig. 5). Standard deviation of the values across all structures for each upper integration limit is provided in the lowest row. The limit of 3.75 eV (the obtained value of the SLRF point) is accompanied by a drop in standard deviation down to 10^{-8}, which falls within accuracy limits for numerical integration.

Structure	0...1 eV	3 eV	3.75 eV	...5 eV
001111100	7.5531	16.4036	19.0000	22.8568
010111100	7.5526	16.3991	19.0000	22.8593
100111100	7.5481	16.3982	19.0000	22.8582
110011100	7.5207	16.4016	19.0000	22.8574
010111010	7.5890	16.3991	19.0000	22.8600
100110011	7.5177	16.4048	19.0000	22.8592
100111001	7.5198	16.4017	19.0000	22.8512
110010011	7.5373	16.3996	19.0000	22.8603
101010101	7.5880	16.3982	19.0000	22.8657
Std. deviation	0.027	0.0045	8×10^{-9}	0.0038

In this sense, the results obtained resemble already known constraints on the DOS like the Barnett-Loudon sum rule (13). However, in the relations obtained in this work the integration involved is *finite* rather than infinite. For the optical case, this means a tighter restriction on the spectral redistribution of the DOS. The compensation of suppression snd enhancement must occur within the frequency interval ω_0. This interval is determined solely by the elementary constituent element of the structure in question [see Eq. (2)]. It is totally independent of geometrical arrangement of these elements. In other words, the QW condition (2) enforces the existence of certain points in the spectrum (the SLRF points) that cannot be "transcended" by electromagnetic states that are "pushed around" the spectrum by layer rearrangement.

On the other hand, the spectral properties of the structure can be arbitrary everywhere between the SLRF points (3). It should also be noted that the increase of N causes the details in the spectra to become finer, and the variation of $T(\omega)$ and $\rho(\omega)$ to get more rapid. These results can help to understand the underlying physics of complex media.

Similar conclusions can be formulated for a quantum par-

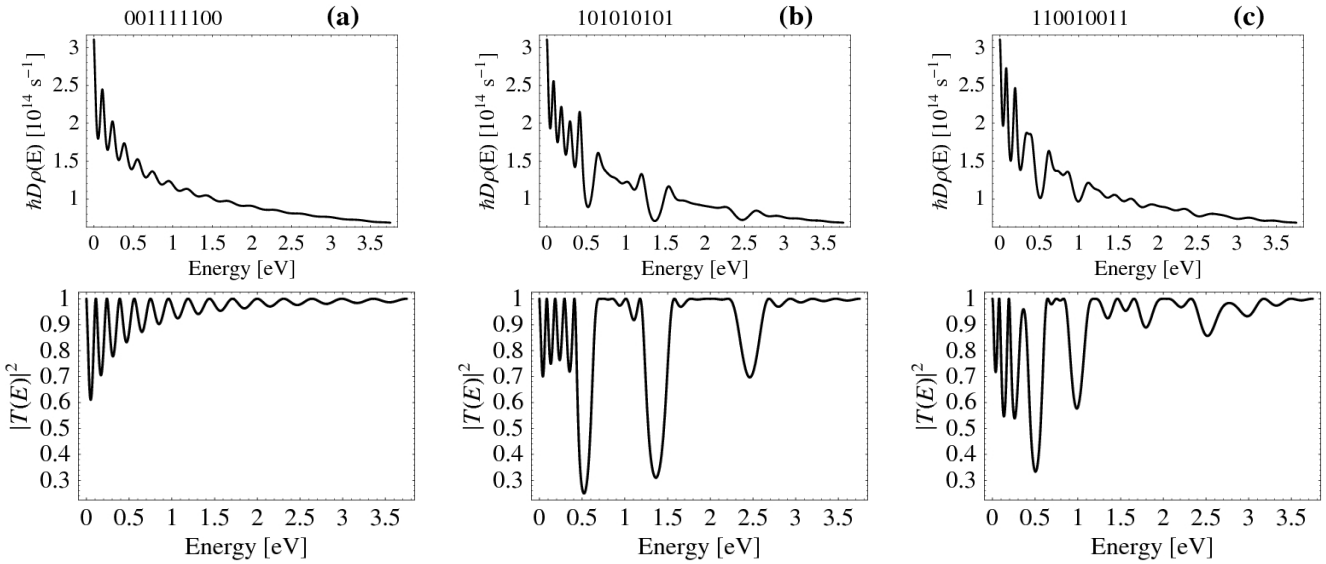

Figure 5: The quantum averaged DOS $\rho(E)$ (top) and transmittance $\left|T(E)^2\right|$ (bottom) for an AlAs/GaAs quantum well and $\beta = 4/5$ in three stepwise potential wells differing only by the elementary well rearrangement: **(a)** single-layer structure; **(b)** periodic structure; **(c)** non-periodic structure. The portion between the SLRF points [0...3.75 eV] is depicted, which corresponds to a solution of Eq. (26) for $j_{\text{qw}} = 1$, $j_0 = 2$, $j_1 = 4$.

ticle in a stepwise potential barrier. However, the inherent quadratic dispersion as seen in Eqs. (8) and (22) results in many differences. First and foremost, the SLRF points are no longer guaranteed. Not only a relative restriction on constituent elements (25) analogous to the QW condition (2) is required, but also individual constraints on $u_{0,1}$ and $d_{0,1}$ are necessary, so as to provide special values of β as determined by Eq. (26). This makes the binarity of the structure an important requirement in contrast to the optical case where Eqs. (2) and (23) can be extended to as many kinds of constituent elements as needed. Because the equation (26) is quadratic rather than linear, the SLRF points occur far more seldom than in the optical case and are no longer equidistant. However, they still do occur on a regular basis if they occur at all for a given choice of parameters, as seen in Fig, 4. In this way, we have provided a way for engineering an electronic heterostructure where the DOS modification due to structure complexity is confined in a finite spectral region. The structure itself can be arbitrarily complex because Eqs. (24)–(26) do not depend on N in any way.

To conclude this section, let us note that the structures in question appear to possess other conservation relations. As can be seen, e.g., in Fig. 2a–c, the transmission spectra contain the same number of resonance peaks in the interval $[0; 2\omega_0]$, namely, nine, which equals the number of constituent layers. Bearing a loose resemblance to the energy level splitting in solids if one regards the layers as "atoms", this was found to be a general property of such multilayers [16]. However, additional restrictions on the structures seem to be necessary, such as the outermost layers of the structure being 1 rather than 0 (compare, e.g., Figs. 2d, e). This requires additional investigations and remains a subject for further studies.

VII. CONCLUSIONS AND OUTLOOK

To summarize, we have investigated the possible degree of modification to transmission and dispersion properties, as well as the averaged local DOS, in discretely inhomogeneous media. Both electromagnetic waves propagating in a dielectric multilayer structure and a quantum particle propagating over a stepwise, multiple-well potential barrier, have been considered (Fig. 1). In both cases, certain constraints on the constituent elements of the structure [Eqs. (2) and (25)] allow to derive the conservation relations over finite frequency or energy regions [Eqs. (17)–(20) and (28), respectively]. Both relations hold *regardless* of the structure geometry (at least in the sense of rearrangement of constituent elements) and are, in this sense, universal, despite the fact that the spectral properties *themselves* can be strongly geometry-dependent. The quantum case appears to be more complicated than the optical one and requires more conditions to be fulfilled, as implied by a quadratic character of Eq. (26). The analytical results obtained have been verified by numerical calculations (see Figs. 2, 5, and Table II).

The results obtained contribute to understanding the physics of complex inhomogeneous media. They can be applied in the design of heterostructures with engineered dispersion, such as chirp compensation, pulse compression or delay line devices. A more detailed studies of the relations obtained would also be useful. It would be of interest to find out if, and to what extent, the results can be applied to the case of optical multilayers made of dispersive and/or absorptive materials, as well as for potential barriers in the tunneling regime.

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